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THE DETONATION VELOCITY-LOADING DENSITY RELATION FOR SELECTED EXPLOSIVES AND MIXTURES OF EXPLOSIVES

BY DONNA PRICE

RESEARCH AND TECHNOLOGY DEPARTMENT

26 AUGUST 1982

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Recent detonation velocity (D) - loading density (ρ_o) data for pure explosives have been reviewed and preferred linear D-ρ_o curves selected. These were then used to predict D of mixtures at densities of 1.0 and 1.6 g/cm^3. The additivity law used was quite successful in both ranges with the exception of high porosity PETN mixtures. The Urizar method of prediction was satisfactory in the low porosity range, but unacceptable in the high porosity range for both pure and mixed high explosives (HE). The Kamlet method was satisfactory for 13 of 15 HE at ρ_o = 1.6 g/cm^3 and for 10 of 15 at ρ_o = 1.0 g/cm^3

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FOREWORD

This report was prepared under Task ZR0000101, IR-59 and OMN funds. It is concerned with the relationship between infinite diameter detonation velocity and loading density of high explosives and mixtures of high explosives. Methods for predicting the velocity of the latter are also considered. The results should be of interest to the areas of detonation chemistry and physics; they are also relevant to the fields of safety and sensitivity.

Approved by:

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Energetic Materials Division

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THE DETONATION VELOCITY-LOADING DENSITY RELATION FOR SELECTED EXPLOSIVES AND MIXTURES OF EXPLOSIVES

INTRODUCTION

For many years, it has been accepted that detonation velocity (D) is a linear function of the loading density (ρ_0) in the range $\rho_0 \geq 1$. Indeed, in 1945, Hurwitz[1] published linear relations derived from the extensive ERL data for numerous explosives. His straight lines were drawn through data of charges prepared from the finest particle size HE and with the largest diameter at $\rho_0 \geq 0.8$ g/cm^3. Hurwitz's values of slopes and intercepts have withstood the test of time very well; they are quoted in at least two texts[2,3] and in many reports. However in 1961, it was reported that the D vs ρ_0 curve of TNT[4] showed a sharp change in slope at $\rho_0 = 1.5324$ g/cm^3. About nine years later, a similar change in slope was reported in the curve for PETN[5] at $\rho_0 = 1.65$ g/cm^3.

There is a possible explanation for this deviant behavior, and one objective of this work is to point it out. A second is to find an acceptable way to predict the detonation velocity of a porous mixture from a knowledge of $D(\rho_0)$ of the components. Finally, the predictions will be compared with experimental values and with approximations obtained by several methods.

In efforts to obtain high density pressed charges, some investigators have used heated molds or solvents or both in the pressing procedure. In general, there is no record of how this would make the charge behavior differ from that of the more widely used cold-pressed charges. In particular, it may increase the critical diameter d_c and hence the diameter effect on D of any size charge. These effects would be expected for HE such as TNT and PETN

---

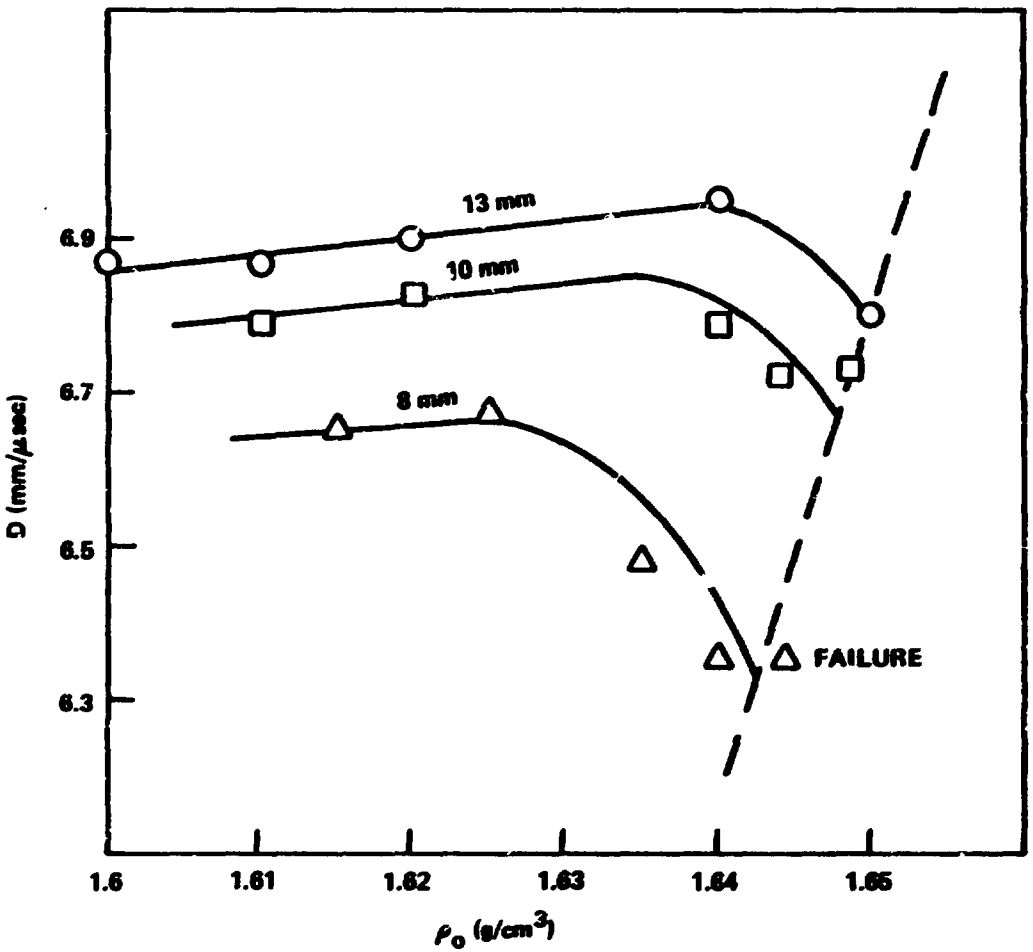
[1] Hurwitz, M. D., "The Rate of Detonation of Various Explosive Compounds and Mixtures," OSRD 5611 (1945).

[2] Cook, M. A., The Science of High Explosives (New York: Reinhold, 1958).

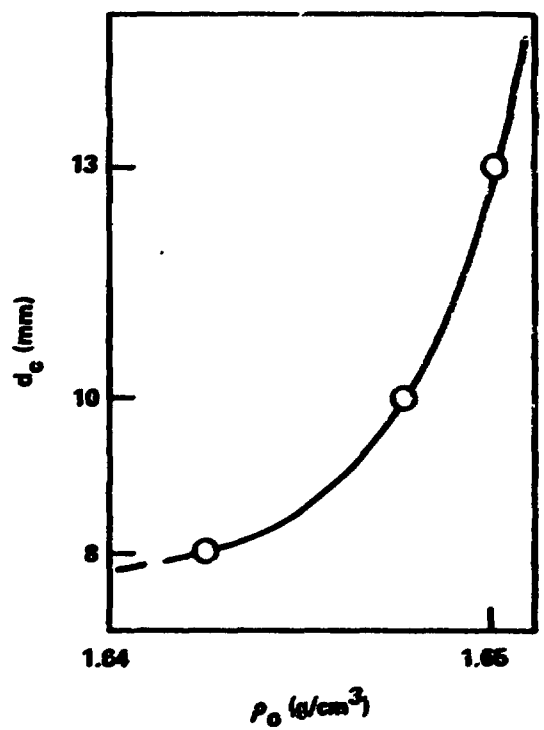
[3] Johansson, C. H., and Persson, P. A., Detonics of High Explosives (New York: Academic Press, 1970).

[4] Urizar, M. J., James, Jr., E., and Smith, L. C., "Detonation Velocity of Pressed TNT," Phys. Fluids, Vol. 4, No. 2, 1961, pp. 262-274.

[5] Hornig, H. C., Lee, E. L., Finger, M., and Kurrle, J. E., "Equation of State of Detonation Products," Proc. 5th Symposium (Int.) on Detonation, ONR ACR-184 (Washington, D. C.: U.S. Gov. Print. Office, 1972), pp. 503-512.



a. D vs ρ_o AT VARIOUS CHARGE DIAMETERS



b. CRITICAL DIAMETER vs CHARGE DENSITY

FIGURE 1 DETONATION BEHAVIOR OF HOT-PRESSED TNT (REF 8)

which flow easily under pressure. Rempel[6] has demonstrated the effect for TNT pressed at 72-76°C in the presence of a little acetone. Figure 1 illustrates it for 8-13 mm dia charges. Since Fig. 1 shows the trend d_c increasing with increasing ρ_o, the opposite of that found for cold pressed charges[7], it is reasonable to suppose that the hot-pressing (aided by solvent) has not only increased ρ_o but also considerably changed the physical nature of the charge. This is particularly likely in view of the low melting point of TNT (80.5°C). In other words the very low porosity, hot-pressed charges approach a cast TNT rather than a cold pressed one in their structure. While it has not been established that cast and pressed TNT differ in D, it has been reported that at ~30 mm dia and ρ_o = 1.62 g/cm^3 the cast TNT has a detonation velocity about 50 m/s lower than the cold pressed[8,9].

---

[6]Rempel, G. G., "Density Dependence of the Critical Diameter and Detonation Velocity of Explosive Charges," PMTF Vol. 10, No. 2, 1969, pp. 83-86, through a translation journal.

[7]Price, D., "Critical Parameters for Detonation Propagation and Initiation of Solid Explosives," NSWC TR 80-339, Sep 1981.

[8]Stesik, L. N., and Akimova, L. N., "An Indirect Method of Estimating the Reaction Zone Width of a Detonation Wave," Russian J. Phys. Chem., Vol. 33, No. 8, 1959, pp. 148-151.

[9]Gibbs, T. R., and Poplato, A., eds., LASL Explosive Property Data (Berkeley: U. Cal. Press, 1980).

SINGLE EXPLOSIVES

TNT

Ref. 4 reports what are probably the most precise detonation velocities measured for TNT. However, all charges of $\rho_0 > 1.44$ g/cm^3 were made by hot-pressing (~70°C). The equation derived for infinite diameter or ideal detonation velocity in the range $\rho_0 \geq 0.9$ g/cm^3 was

$$D_i(\text{mm}/\mu\text{s}) = \begin{cases} 1.8727 + 3.1872\ \rho_0 & 0.9 \leq \rho_0 \leq 1.5342 \\ 6.7625 + 3.1872\ (\rho_0 - 1.5342) & \\ \quad - 25.102\ (\rho_0 - 1.5342)^2 & \\ \quad + 115.056\ (\rho_0 - 1.5342)^3 & 1.5342 \leq \rho_0 \leq 1.636\ \text{g/cm}^3 \end{cases} \quad (1)$$

Recent handbooks[9,10] quote Eq. 1 without the cubic term or any comment on its absence.

Fig. 2 compares Eq. 1 with that derived by Hurwitz:[1]

$$D_i = 1.785 + 3.225\ \rho_0 \quad (2)$$

Each curve has been terminated at the highest experimental density reported. The two sets of results are within experimental error except at the higher densities where hot-pressed charges were used. There Eq. 1 indicates a sharp decrease in the slope; that could result from an increased critical diameter such as shown in Rempsel's data. An increased d_c would increase the diameter effect on the measured detonation velocity at any given diameter and hence might result in $D_{measured} < D_i$.

---

[10] Dobratz, B. M., ed., LLNL Explosives Handbook, UCRL-52997, 1981 with 1982 addenda.

[11] Campbell, A. W., and Engelke, R., "The Diameter Effect in High Density Heterogeneous Explosives," Sixth Symposium (Int.) on Detonation, ONR ACR 221, (Washington, D. C.: U. S. Gov. Print. Office, 1978) pp. 642-663.

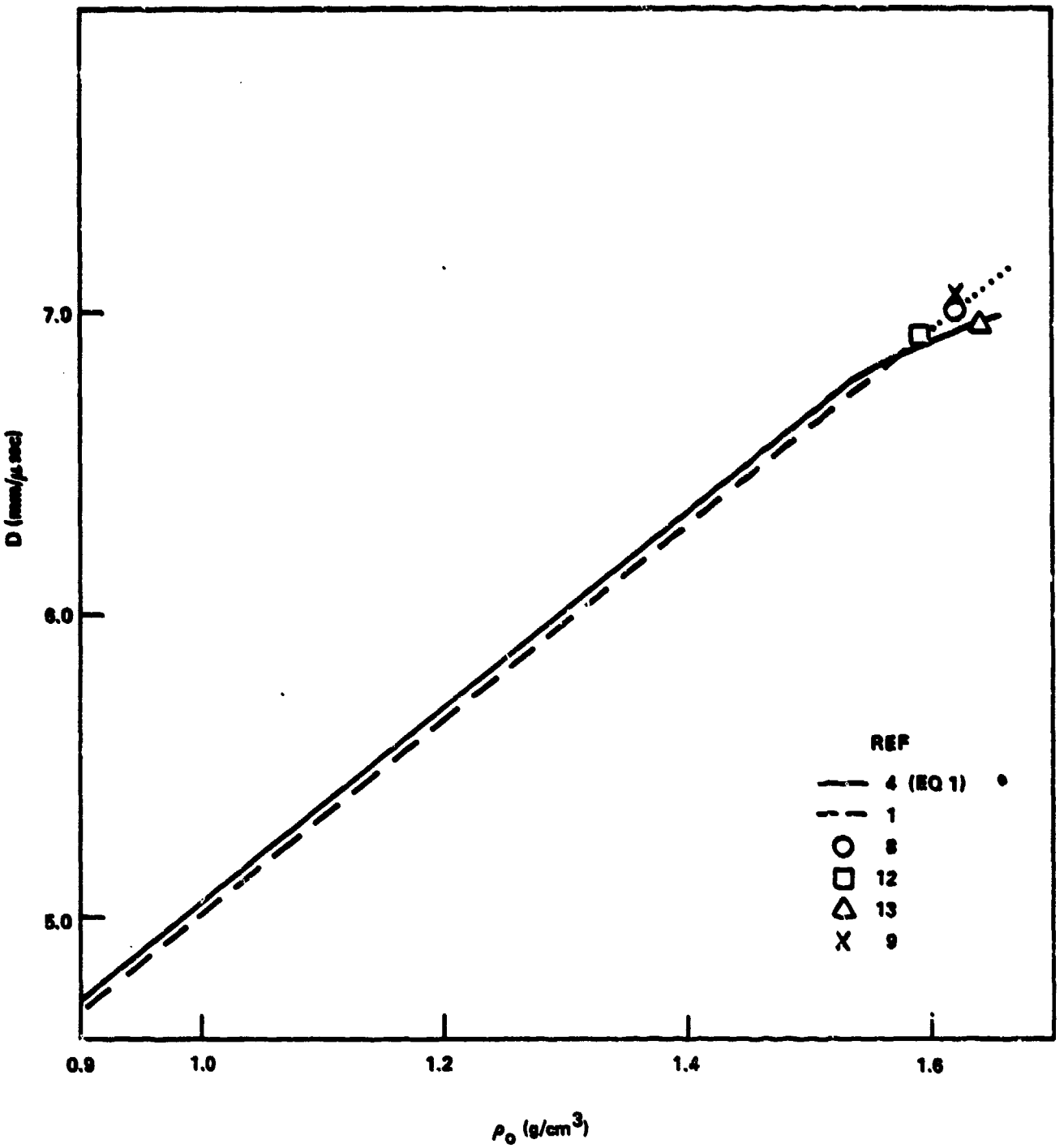


FIGURE 2 D (ρ_o) CURVES AND DATA FOR TNT

Ref. 9, in addition to Eq. 1 without the cubic term, also quotes 7.045 mm/μs* as D_j for pressed TNT at ρ_o = 1.620 g/cm^3. However Eq. 1 produces D_j(1.620 g/cm^3) = 6.924 mm/μs (6.051 mm/μs if cubic term omitted).

If the change in slope shown by Eq. 1 is ignored, the relation becomes

$$D_j = 1.8727 + 3.1872\ \rho_o \qquad \rho_o \geq 0.9\ \text{g/cm}^3 \qquad (3)$$

Moreover, for ρ_o = 1.62 g/cm^3, Eq. 3 produces D_j = 7.036 mm/μs, in quite good agreement with the 7.045 mm/μs value. Typical high density experimental values of (D_j,ρ_o) are: (7.00,1.62)[8], (6.91,1.59)[12], and (6.91,1.64);[13] the first two sets are Russian, the last from LANL (hot-pressed charge). These points are also plotted in Fig. 2 to demonstrate the pattern of Russian data failing to exhibit the change of slope at high density. NSWC has obtained TNT at 1.60 g/cm^3 by pressing cold charges in the hydraulic press and at 1.64 g/cm^3 in the isostatic press. It seems possible and even likely that the Russian data[8,12] were obtained by pressing cold charges. In view of the possible effect of hot-pressing on the charge performance, it is suggested that Eq. 3 be used for cold-pressed charges. It will be so used with the prediction method for mixtures described later. Of course, an experimental investigation of the measurable effects on d_c and D(d) of hot-pressed vs cold-pressed charges is strongly recommended as well.

PETN

PETN has a higher melting point than TNT (141°C), but it too flows easily under pressure. The most precise D measurements on PETN are probably those of Ref. 5. That reference did not state whether the pressing was of cold or heated PETN. However, LLNL generally uses hot-pressing as does LANL.

Ref. 5 presents the D_j vs ρ_o curve as

$$D_j(\text{mm/μs}) = \begin{cases} 2.14 + 2.84\ \rho_o & \rho_o < 0.37\ \text{g/cm}^3 \\ 3.19 + 3.70\ (\rho_o - 0.37) & 0.37 < \rho_o < 1.65 \\ 7.92 + 3.05\ (\rho_o - 1.65) & \rho_o > 1.65 \end{cases} \qquad (4)$$

---

[12] Dremin, A. N., and Shvedov, K. K., "Determination of C-J Pressure and Reaction Duration in the Detonation Wave of HE," PMTF No. 2, 1964, pp. 154-159, through a translation.

[13] Mader, C. L., Los Alamos Rept. LA-2900, 1963.

*This value was derived from Ref. 8 after smoothing the function D(d) according to the method of Ref. 11.

In the intermediate density range of 1.0 ± 0.2 g/cm^3, Eq. 4 and Refs. 1, 14, and 15 are in very close agreement. Ref. 1 limits its data to $\rho_o \geq 0.8$ g/cm. Below that limit, Refs. 14 and 15 are still in good agreement with Eq. 4 provided their data are forced to extrapolate to the theoretical value[16] of 2.19 mm/μs at $\rho_o = 0.01$ g/cm^3; that value compares well with 2.17 mm/μs at $\rho_o = 0$ from Eq. 4. It was probably the difficulty of obtaining uniform and stable charges at $\rho_o \leq 0.5$ g/cc that resulted in reported D measurements at very low ρ_o well above the Eq. 4 curve in Ref. 14.

In the range $\rho_o \geq 0.95$ g/cm^3, Eq. 4 is shown as the dashed line of Fig. 3. Also shown is the curve

$$D_i = 1.600 + 3.950\ \rho_o \qquad (5)$$

from Ref. 1. Ref. 5 quotes six experimental values attributed to a report by E. A. Christian and H. G. Snay. However, those values were all derived from Eq. 5. Table 1 contains the additional experimental data plotted in Fig. 3. They are in good agreement with Eq. 4 up to $\rho_o = 1.65$ g/cm^3. Above that density, LANL data lie below and the Russian data lie above the Eq. 4 curve.* For the same reasons considered in the case of TNT, it is suggested that the equation

$$D_i = 1.82 + 3.70\ \rho_o \qquad \rho_o \geq 0.8\ \text{g/cm}^3 \qquad (6)$$

be used for computing D of mixtures containing PETN.

Other Pure HE

Other single explosives to be considered here are BTNEU, DINA, RDX(HMX), tetryl and TNETB.

BTNEU, bis(trinitroethyl) urea, $O{=}C[(NHCH_2C(NO_2)_3]_2$ is a high energy, sensitive explosive with a voidless density of 1.86 g/cm^3 and a decomposition

[14] Friederich, W., "Über die Detonation der Sprengstoffe," Z. ges. Schiess-Sprengstoffw., Vol. 28, 1933, pp. 2-6, 51-3, 80-3 and 113-16.

[15] Paterson, S., Teknick-Vetenskaplig Forskning, Vol. 29, 1958, pp 109-120. The same data are quoted in the text, J. Taylor, Detonation in Condensed Explosives (Oxford: Clarendon Press, 1950).

[16] Stesik, L. N., and Shvedova., N. S., "Detonation of Condensed Explosives with Low Charge Densities," PMTF, No. 4, 1964, pp. 124-126, ONI translation No. 2111.

*It is of interest that the LANL curve for PETN[9]

$$D = 1.608 + 3.933\ \rho_o \qquad 0.57 < \rho_o < 1.585$$

extrapolates to 8.49 mm/μs at $\rho_o = 1.75$ g/cm^3. This value lies quite close to the Russian data. Of course, this is also true of Eq. 6.

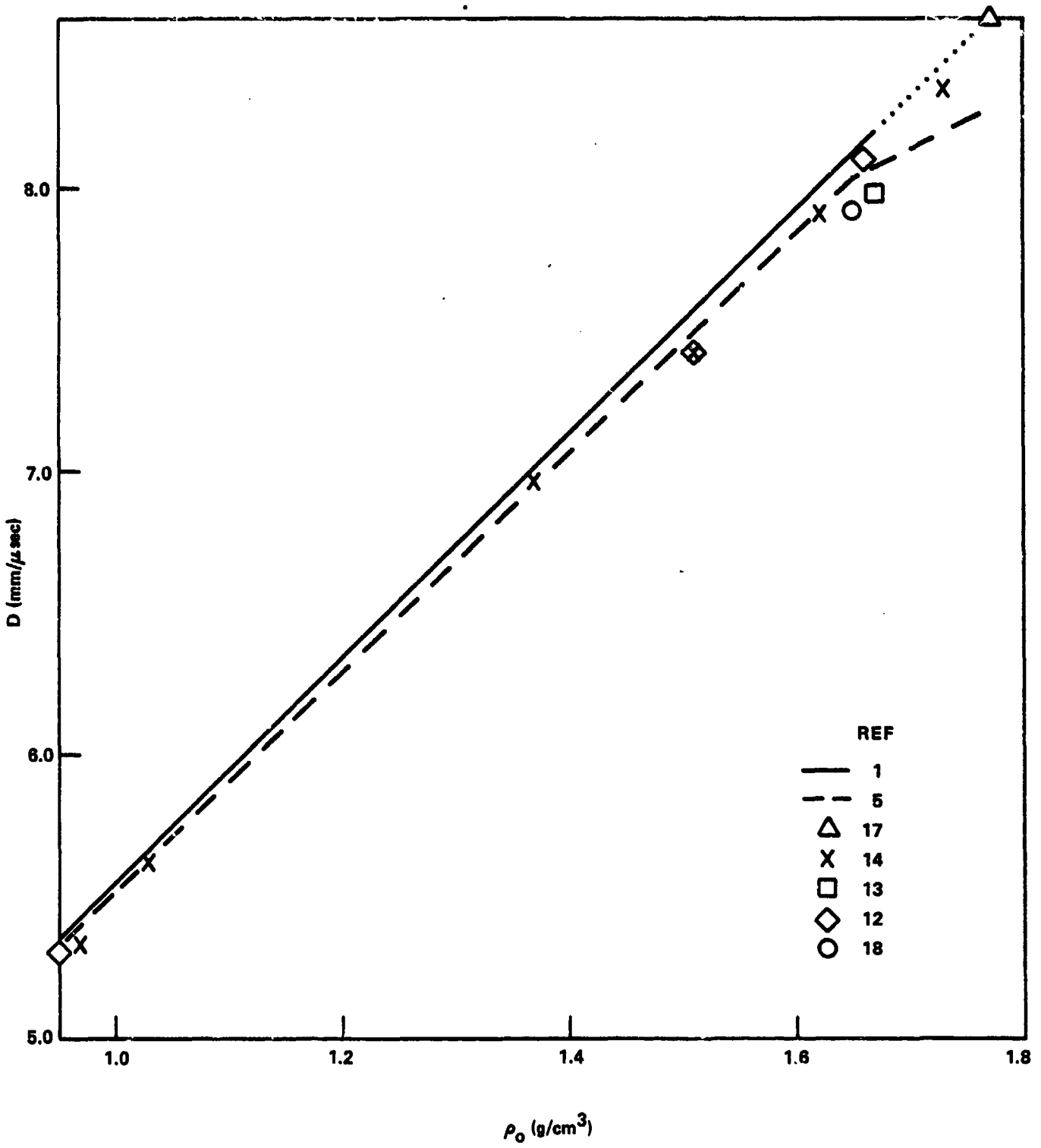


FIGURE 3 D (ρ_o) CURVES AND DATA FOR PETN

TABLE 1

Experimental Values for $D_i(\rho_o)$ of PETN in Range $\rho_o \geq 0.95$ g/cm^3

ρ_o g/cm^3	D mm/μs	Ref.
1.77	8.60	17
1.73	8.35	14
1.67	7.98	13
1.66	8.10	12
1.65	7.92	18
1.62	7.91	14
1.51	7.42	12
1.51	7.42	14
1.37	6.97	14
1.03	5.62	14
0.97	5.33	14
0.95	5.30	12

[17] Apin, A. Ya., and Voskoboynikov., I. M., "Calculation of Parameters of a Detonation Wave of Condensed Explosives," PMTF, No. 4, 1960, pp. 54-55, ONI Translation No. 2083.

[18] Craig, B., through Ref. 5.

point of ∿186°C. Its D_i was derived from experimental measurements in Refs. 19 and 20:

$$D_i = 1.42 + 4.08\rho_o \quad (7)$$

The charges used were highly porous or contained 2% wax as a binder at ∿1.6 g/cm^3. However Eq. 7 extrapolates to within 0.1% of the value measured at 1.86 g/cm^3 in small scale (confined) charges.

DINA, diethanolnitramine dinitrate, $O_2N\text{-}N(CH_2CH_2ONO_2)_2$ has a voidless density of 1.67 g/cm^3 and m.p. of 52.5°C. It is an easily synthesized, easily castable energetic explosive, and has been used in DDT studies. Ref. 1 gives for this HE

$$D_i = 3.00 + 2.95\rho_o \quad (8)$$

A review has been made of the data available since Ref. 1 was published. These data are collected in Table 2 and plotted in Fig. 4. Measured D for cast DINA was included because Ref. 1 showed that its measured velocity fell on the curve obtained with pressed charges.

The solid line of Fig. 4 is a least squares fit to the eight data pairs of Table 2. Its equation is

$$D_i = 3.03 + 2.93\rho_o \quad (9)$$

with σ = 0.66 mm/μs. There is consequently no justification for changing Eq. 8, particularly since it treats a greater amount of data from charges prepared by standardized methods at ERL.

RDX(HMX) share the same $D(\rho_o)$ function which is

$$D_i = 2.56 + 3.47\rho_o \quad (10)$$

from Ref. 10. This equation fits the RDX mixtures data at ρ_o = 1.0 g/cm^3 better than that in Ref. 9 although both give equivalent values at voidless density. It was demonstrated some time ago that the low porosity LANL data[9]

---

[19]August, W. T., Liddiard, T. P., Lovenberg, C. C., Shapiro, N., Solem, A. D., Stresau, R. H., and Svadeba, G., "Evaluation of BTNEU as a Substitute for RDX," NavOrd 2287, Dec 1951.

[20]Coleburn, N. L., and Liddiard, T. P., "The Rates of Detonation of Several Pure and Mixed Explosives," NavOrd 2611, Sep 1952.

TABLE 2

$D_i(\rho_o)$ Data Recently Reported for DINA

ρ_o g/cm^3	D mm/μs	Ref.
1.67	8.00	17
1.64	7.80	21
1.60 c*	7.72	22
1.60	7.73	23
1.55	7.58	23
1.48	7.40	17
1.36	7.00	21
0.95	5.80**	21

[21]Dremin, A. N., Savrov, S. D., Trofimov, V. S., and Shvedov, K. K., Detonation Waves in Condensed Media (Moscow: Izd-vo Nauka, 1970) FTD-HT-23-1889-71 (AD 751417).

[22]Price, D., Jaffe, I., and Toscano, J. P., "Development of the Continuous Wire Method II," NOLTR 66-21, Mar 1966.

[23]Fedoroff, B. T., and Sheffield, O. E., eds., Encyclopedia of Explosives and Related Items, Vol. 5 (Dover, N. J.: Picatinny Arsenal, 1972), p. D-1241.

*Only charge for which preparation data are available.

**Value given in translation used is 5.08. However, this is clearly a typographical error as can be checked with values of detonation pressure and particle velocity that are also listed.

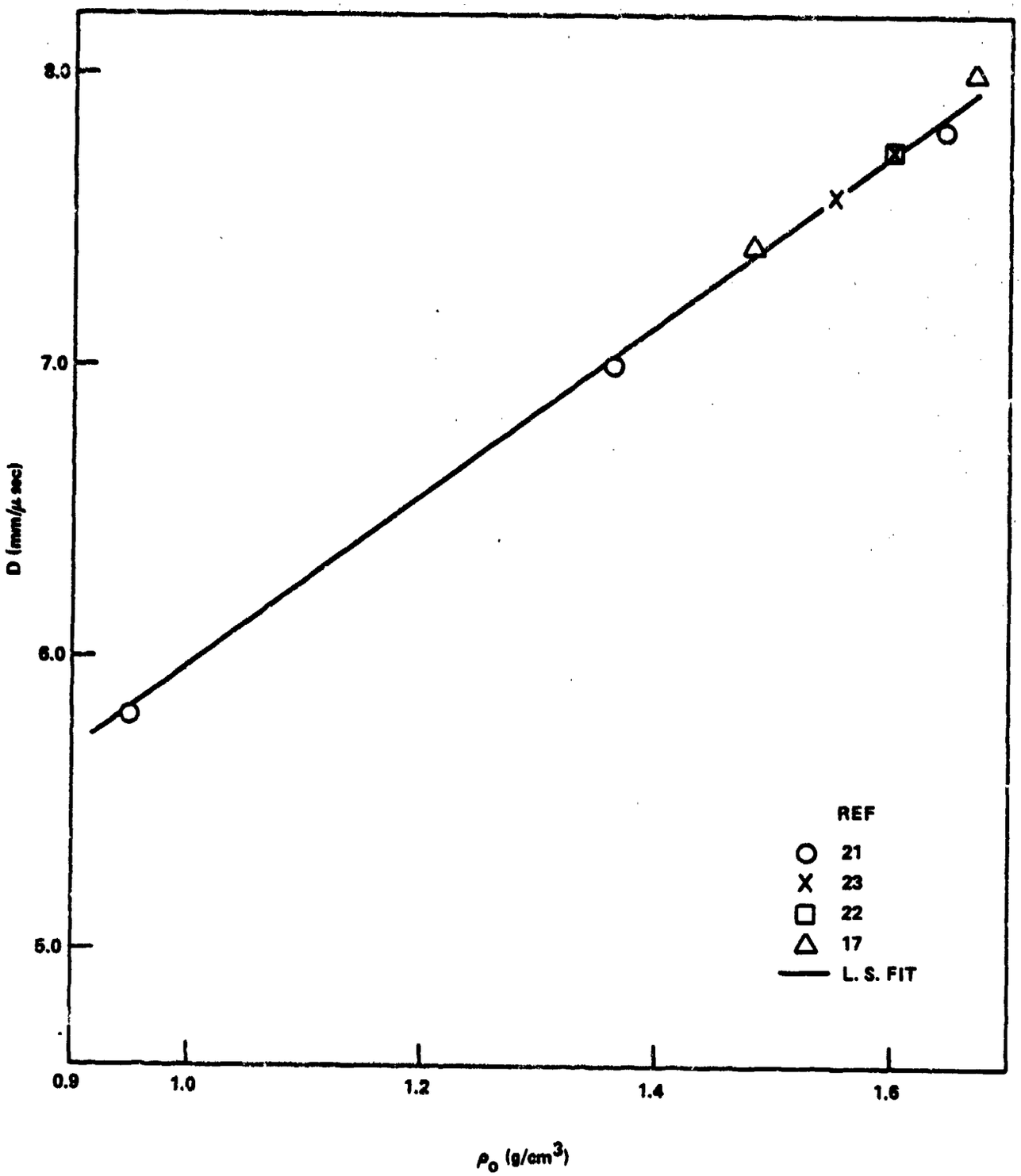


FIGURE 4 D vs ρ_o DATA RECENTLY REPORTED FOR DINA

(and hence the low porosity LLNL data[10]) for RDX were more consistent than those of NSWC.[24]

Tetryl is another important commercial explosive for which the $D(\rho_0)$ function does not seem to have been reexamined since 1945[1]. The relation given in Ref. 1 is

$$D_j = 2.375 + 3.225\rho_0 \tag{11}$$

On the other hand, Ref. 9 gives

$$D_j = 2.742 + 2.935\rho_0 \qquad 1.3 \leq \rho_0 \leq 1.69 \tag{12}$$

which is appreciably different from Eq. 11. Table 3 contains some of the more recent data for tetryl, and Fig. 5 displays them together with Eqs. 11 and 12. It is evident that the data conform better to Eq. 12 than to Eq. 11; hence the former will be used for mixtures. Ref. 21 values seem to run a bit low and Ref. 17, a bit high as they did for DINA. Aside from that, the larger discrepancies at low porosity might arise from different methods of charge preparation, different instrumentation, or both.

TNETB, trinitroethyltrinitrobutyrate, $(NO_2)_3CCH_2CH_2COOCH_2C(NO_2)_3$, is a castable (m.p. 93°C) high energy explosive. Since its $D(\rho_0)$ function, as reported in the 1965 NSWC Explosives Handbook, is somewhat in error, the corrected function is presented here for convenience; its derivation was reported in TR 68-182.

$$D_j = 1.947 + 3.660\rho_0, \ \sigma = 0.015 \text{ mm/}\mu\text{s} \tag{13}$$

Eq. 13 is very similar to Eq. 6, the analogous relation for PETN.

---

[24] Price, D., "Inter-relationship of Explosive Characteristics III," NavOrd 4510, Apr 1957.

TABLE 3

Additional $D_i(\rho_o)$ Data for Tetryl

ρ_o g/cm^3	D_i mm/μs	Ref.
1.71	7.85	10
1.70	7.860	17
1.70	7.560	13
1.68	7.50	21
1.614	7.581	25
1.60	7.400	23
1.55	7.30	23
1.51	7.17	26
1.506	7.150	27
1.44	6.875	28
1.36	6.68	21
1.22	6.291	14
0.9-0.95	5.36	21
0.95	5.390	28

---

[25]Coleburn, N. L., "C-J Pressures of Several Pure and Mixed Explosives," NOLTR 64-58, Sep 1964.

[26]Clairmont, A. R., and Jaffe, I., "Analysis of the Optical Determination of Detonation Velocity in Short Charges," NOLTR 64-23, May 1964.

[27]Cybulski, W. B., Payman, W., and Woodhead, D. W., Roy. Soc. London Proc., Vol. 197A, 1949, pp. 51-72.

[28]Woodhead, D. W., and Titman, H., "Detonation Phenomena in a Tubular Charge of Explosive," Explosivstoffe, Vol. 5, 113-123 and 6, 141-155, 1965.

[29]Price, D., Clairmont, Jr., A. R., Erkman, J. O., and Edwards, D. J., "Ideal Detonation Velocity of Ammonium Perchlorate and its Mixtures with HE," NOLTR 68-182, Dec 1968.

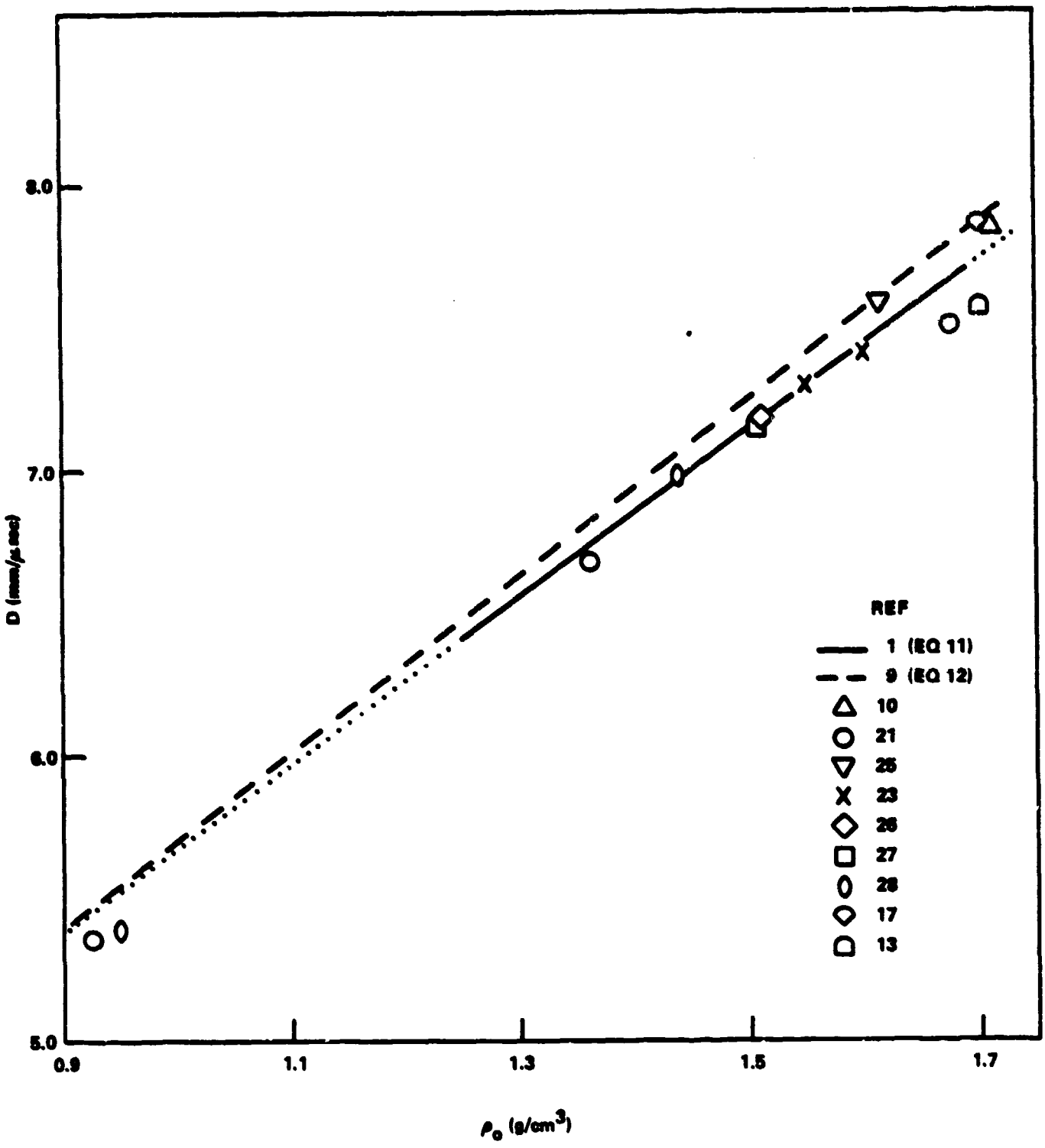


FIGURE 5 D (ρ_o) CURVES AND DATA FOR TETRYL

MIXTURES OF HE

The experimental values of the mixed HE will be obtained from the curves reported by Coleburn and Liddiard[20]. In general, deriving such curves results in averaging and compensating for errors introduced by unrecognized differences in charge preparation, measurements, and record reading. Thus a velocity value on a D-ρ_0 curve derived from a number of experimental values over the density range is considered of equal or greater accuracy than the individual experimental values upon which it is based. (Similarly an average of two or more experimental measurements on charges of the same density is considered to be more accurate than individual measurements.) This is also considered to be the case for pure explosives.

Table 4 contains a summary of the $D(\rho_0)$ functions chosen for the single HE and those given in Ref. 24 for the mixtures. All are in the form

$$D_i = a + b\rho_0 \tag{14}$$

In addition to a and b, the intercept and the slope, ρ_c (the voidless or theoretical maximum density or TMD) is also listed. Eq. 14 can be rearranged to

$$D_i = a + b\rho_c\Delta \tag{15}$$

where

$$\Delta = \rho_0/\rho_c = \%TMD/100$$

For this reason, $b\rho_c$ is also listed in Table 4.

In addition, Table 4 contains the curves derived from the data of Ref. 20 for mixtures of HE. Only three of the mixtures are included in the Ref. 1 compendium: pentolite, cyclotol 60/40 (Ref. 1 does not distinguish between this cyclotol and Comp B) and tetrytol 70. In the first two cases, the curves were essentially the same i.e., less than 1% difference for pentolite and 1 - 1.4% difference for the cyclotol; the Ref. 20 data gave higher values, possibly because Comp B (Ref. 1) includes 1% wax. However, the two tetrytol curves differed significantly (ca. 5% at 1 g/cm^3 - not as much at higher densities.) The curve from Ref. 20 was used.

Table 4 Detonation Velocity of HE Mixtures Estimated by Additivity, Equation 17

HE	ρ_c g/cm^3	a mm/μs	b $\frac{cm^3}{g}\frac{mm}{\mu s}$	$b\rho_c$ mm/μs	ρ_o = 1 g/cm^3 %TMD	D_{exp}	D_{calc}	% Diff.	ρ_o = 1.6 g/cm^3 %TMD	D_{exp}	D_{calc}	% Diff.
BTNEU	1.86	1.42	4.08	7.59								
DINA	1.67	3.00	2.95	4.93								
HMX	1.902	2.56	3.47	6.60								
PETN	1.78	1.82	2.70	6.59								
RDX	1.806	2.56	3.47	6.27								
Tetryl	1.73	2.742	2.935	5.08								
TNETB	1.78	1.947	3.650	6.51								
TNT	1.654	1.873	3.187	5.27								
		Mixtures*										
BTNEU/TNT 60/40	1.77	1.58	3.81	6.74	56.50	5.39	5.37	-0.4	90.40	7.67	7.62	-0.7
HMX/TNT 74.8/25.2	1.833	2.42	3.33	6.10	54.56	5.75	5.80	+0.9	87.29	7.74	7.86	+1.6
Pentolite 50/50	1.71	2.33	3.17	5.42	58.48	5.50	5.31	-3.5	93.57	7.40	7.40	0.0
PTX-2	1.75	2.57	3.23	5.65	57.14	5.80	5.62	-3.1	91.43	7.74	7.71	-0.4
PETN/RDX/TNT 28/43.2/28.8	1.74	2.59	3.16	5.50	57.47	5.75	5.66	-1.6	91.95	7.65	7.68	-0.4
RDX/TNT 60/40	1.77	2.54	3.29	5.82	56.50	5.83	5.79	-0.7	90.40	7.80	7.83	+0.4
RDX/TNT 75/25	1.71	2.80	2.75	4.70	58.48	5.55	5.49	-1.1	93.57	7.20	7.29	+1.3
Tetryl/TNT 70/30							Av. abs. error	-				0.7%
								1.6				

*Values from Ref. 20.

(0.9% without PETN mixes)

To predict D_i for a mixture from known $D_i(\rho_o)$ of the components, the additivity relation

$$D_i(\rho_o)_{mix} = \sum_j x_j D_j , \tag{16}$$

where x_j is weight fraction of component j and D_j is the ideal detonation velocity of component j at the porosity of the mixture, was suggested some time ago[29]. It was at that time applied only to materials at voidless density; for the present application it has been generalized to any porosity in the linear range of the $D(\rho_o)$ functions. Eq. 15 in conjunction with Eq. 15 produces the predictive equation

$$D_i(\rho_o)_{mix} = \sum x_j \left[a_j + b_j \rho_{cj} \left(\frac{\rho_o}{\rho_c} \right)_{mix} \right] \tag{17}$$

Eq. 17 has been used to predict the detonation velocity of mixtures at densities of 1.0 and 1.6 g/cm^3. The predicted and observed values are listed in Table 4.

About forty years ago, Urizar formulated an empirical equation for predicting detonation velocity from a knowledge of detonation velocity at crystal density (D_c) of each mixture component. His expression, described on p. 8-10 of Ref. 10 is

$$D_i(\rho_o) = \sum_j y_j D_{cj} \tag{18}$$

where y_j is volume fraction of component j. For non-explosive components such as air, Al and NaCl, he gave empirical values for D_c. For air (voids) this empirical number is 1.5 mm/μs.

Since for each solid component,

$$y_j = \rho_o \frac{x_j}{\rho_{cj}} \tag{19}$$

and for the voids

$$y_a = 1 - \sum^{solids} y_j = 1 - (\% \text{ TMD}/100) \tag{20}$$

Eq. 18 becomes

$$D_i(\rho_o) = \rho_o \sum^{solids} \frac{x_j}{\rho_{cj}} (a_j + b_j \rho_{cj}) + 1.5\, y_a \tag{21}$$

Eq. 21 was used to calculate D_i at ρ_o = 1.0 and 1.6 g/cm^3 for both single explosives and mixtures. The experimental and computed values are listed in Table 5.

Table 5 Detonation Velocity of Pure and Mixed HE Predicted by Method of Urizar, Equation 21

HE	ρ_c g/cm^3	D_c mm/μs	ρ_0 = 1.0 g/cm^3 y_1	y_2	y_a	D_{calc}	D_{exp}	% Diff.	ρ_0 = 1.6 g/cm^3 y_1	y_2	y_a	D_{calc}	D_{exp}	% Diff.
BTNEU	1.86	9.01	0.5376		0.4624	5.54	5.50	+0.7	0.8602		0.1398	7.96	7.95	+0.1
DINA	1.67	7.93	0.5988		0.4012	5.36	5.95	-10.1	0.9581		0.0419	7.66	7.73	-0.9
HMX	1.902	9.16	0.5258		0.4742	5.53	6.03	-8.3	0.8412		0.1588	7.94	8.11	-2.1
PETN	1.78	8.41	0.5618		0.4382	5.38	5.52	-2.5	0.8989		0.1011	7.71	7.74	-0.4
RDX	1.806	8.83	0.5537		0.4463	5.56	6.03	-7.8	0.8859		0.1141	7.99	8.11	-1.5
Tetryl	1.73	7.82	0.5780		0.4220	5.15	5.68	-9.3	0.9249		0.0751	7.35	7.44	-1.2
TNETB	1.78	8.46	0.5618		0.4382	5.41	5.61	-3.6	0.8989		0.1011	7.76	7.80	-0.5
TNT	1.654	7.14	0.6046		0.3940	4.91	5.06	-3.0	0.9674		0.0326	6.96	6.97	-0.1
						Av. Abs. Error		5.7%						0.9%
BTNEU/TNT 60/40	1.77	8.32	0.3226	0.2418	0.4350	5.29	5.39	-1.9	0.5161	0.3869	0.0960	7.56	7.67	-1.4
HMX/TNT 74.8/25.2	1.833	8.52	0.3933	0.1524	0.4544	5.37	5.75	-6.6	0.6292	0.2438	0.1271	7.69	7.74	-0.6
Pentolite 50/50	1.71	7.75	0.2809	0.3023	0.4152	5.14	5.50	-4.7	0.4494	0.4837	0.0643	7.33	7.40	-0.9
PTX-2 PETN/RDX/TNT 28/43.2/28/8	1.75	8.22	0.1573	(0.1741)* 0.2392	0.4286	5.32	5.80	-8.3	0.2517	(0.2786)* 0.3827	0.0857	7.61	7.74	-1.7
RDX/TNT 60/40	1.74	8.09	0.3322	0.2418	0.4253	5.30	5.75	-7.8	0.5316	0.3869	0.0805	7.58	7.65	-0.9
RDX/TNT 75/25	1.77	8.36	0.4153	0.1511	0.4350	5.40	5.83	-7.4	0.6645	0.2418	0.0960	7.74	7.80	-0.8
Tetryl/TNT 70/30	1.71	7.50	0.4046	0.1814	0.4152	5.08	5.55	-8.5	0.6474	0.2902	0.0643	7.23	7.20	+0.4
						Av. Abs. Error		6.5%						1.0

*y_3 of PTX-2

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The last approximation, again applicable to either pure HE or their mixtures, to be considered here is that of Kamlet[30]. This approximation is based on the arbitrary decomposition that uses the available oxygen in the HE to form $H_2O(g)$ and CO_2 in that sequence. Then

$$D_j \text{ (mm/μs)} = 1.01\phi^{1/2} (1 + 1.30 \rho_0) \quad (22)$$

where ρ_0 is density in g/cm^3, and $\phi = NM^{1/2} Q_{arb}^{1/2}$; N, M, and Q_{arb} are, respectively, number of moles of gaseous products per gram HE, average molecular weight of gaseous products, and the specific chemical energy of the detonation reaction. The values of N, M, Q_{arb}, and ϕ are all determined by the arbitrary equation used. Again D_j values at ρ_0 = 1.0 and 1.6 g/cm^3 have been computed and are compared to the observed values in Table 6.

The Table 4 data show that the additivity method of Eq. 17 is a very good way to predict velocities of these mixed HE at moderate to low porosities ($\rho_0 \sim$ 1.6 g/cm^3). Its average absolute error is less than 1% and the individual error less than 2%. With the exception of mixtures containing PETN, it is equally effective at high porosity ($\rho \sim$ 1.0 g/cm^3), but the PETN mixtures show errors of up to -3.5%. A possible reason for this is that Eq. 17 assumes no interaction between the detonation products of the low and high oxygen components of the mixtures. At high porosities the reaction time is greater and the reaction temperature higher than at low porosity. Under these conditions interactions, absent at low porosities, might occur and result in increasing the detonation velocity. This possibility seems somewhat probable in view of the fact that the Kamlet method, which assumes complete interaction, is satisfactory for these mixtures at ρ_0 = 1.0 g/cm^3 despite its unsatisfactory result at higher density for the high oxygen component, PETN[30].

As the Table 5 data show, the Urizar method is almost equally acceptable for both pure and mixed HE at $\rho_0 \sim$ 1.6 g/cm^3. It is, however, quite inadequate at high porosities where individual results vary from the experimental by as much as 10% and the average absolute difference is 6-7%.

The Kamlet method (Table 6) gave excellent results for this set of mixtures at ρ_0 = 1.6 g/cm, and, with the exception of the 60/40 BTNEU/TNT, acceptable ones at the higher porosity. However, its prediction for pure explosives was not good at the lower density. With the exception of DINA, the HE showing the higher discrepancies at ρ_0 = 1.6 g/cm^3 exhibited greater discrepancies (up to 10%) at the greater porosity.* Those HE showing

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[30] Kamlet, M. J., and Hurwitz, H., J. Chem. Phys., Vol. No. 48, No. 8, 1968, pp. 3685-3692.

*Comparisons in Tables 4 and 5 are at fixed densities. If instead fixed porosity is used, the picture is the same. E.g., at 57% TMD, instead of ρ_0 = 1 g/cm^3, the single HE show an average absolute error of 5.5 and 3.6%, respectively for values from the Urizar and Kamlet methods.

TABLE 6 Detonation Velocity of Pure and Mixed HE
Predicted by Method of Kamlet, Equation 22

HE	ϕ^*	$\phi^{1/2}$	ρ_o = 1 g/cm^3 D_{calc}	D_{exp}	% Diff.	ρ_o = 1.6 g/cm^3 D_{calc}	D_{exp}	% Diff.
BTNEU	6.783	2.604	6.05	5.50	+10.0	8.10	7.95	+1.9
DINA	6.562	2.562	5.95	5.95	0.0	7.97	7.73	+3.1
HMX	6.772	2.602	6.04	6.03	+0.2	8.09	8.11	-0.2
PETN	6.805	2.609	6.06	5.52	+9.8	8.12	7.74	+4.9
RDX	6.784	2.605	6.05	6.03	+0.3	8.10	8.11	-0.1
Tetryl	5.615	2.370	5.51	5.68	-3.0	7.37	7.44	-0.9
TNETB	6.587	2.567	5.96	5.61	+6.2	7.99	7.80	+2.4
TNT	4.838	2.199	5.11	5.06	+1.0	6.84	6.97	-1.9
			Av. Abs. Error		3.8%			1.9%
BTNEU/TNT 60/40	5.977	2.445	5.68	5.39	+5.4	7.61	7.67	-0.8
HMX/TNT 74.8/25.2	6.283	2.507	5.82	5.75	+1.2	7.80	7.74	+0.8
Pentolite 50/50	5.796	2.408	5.59	5.50	+1.6	7.49	7.40	+1.2
PTX-2								
PETN/RDX/TNT 28/43.2/28.8	6.206**	2.491	5.78	5.80	+0.7	7.75	7.74	+0.1
RDX/TNT 60/40	5.992	2.448	5.69	5.75	-1.0	7.62	7.65	-0.4
RDX/TNT 75/25	6.292	2.508	5.83	5.83	0.0	7.80	7.80	0.0
Tetryl /TNT 70/30	5.379	2.319	5.39	5.55	-2.9	7.21	7.20	+0.1
			Av. Abs. Error		1.8%			0.5%

*Ref. 30.

**Computed

the greatest differences between predicted and observed D were BTNEU, PETN, and TNETB - all high oxygen HE. The discrepancy for PETN was noted in Ref. 30, but no data for high porosity BTNEU and TNETB were considered.* Of course, results of the comparison between predictions by this method and the experimental values will be influenced by the choice made for the experimental curve more than the two earlier comparisons because the other methods are both based on experimental values whereas this one is not.

*In the case of DINA, the experimental data used in Ref. 30 were the Ref. 17 data shown on Fig. 4. The higher density value was well above the curve chosen here for the linear curve; hence the discrepancy observed in Ref. 30 was not as great as the present +3.1%.

SUMMARY

It is suggested that the recently reported sharp changes in slope of the $D(\rho_0)$ curves at nigher densities for TNT[4] and PETN[5] may result from changes in the charges caused by hot-pressing. In other words, the increased homogeneity of the hot-pressed charges can increase the critical diameter and thereby the diameter effect (a lowering of D at finite diameters) on measured detonation velocity. Therefore, it is strongly recommended that the effect of hot-pressing on D be investigated.

$D(\rho_0)$ data for TNT, PETN, BTNEU, DINA, RDX(HMX) and tetryl have been reviewed and a best experimental curve selected in each case. These curves have been used to predict the D values of HE mixtures by an additivity rule. The predicted values were in excellent agreement with the measured values (Ref. 20) at high and low porosities except for two high porosity mixtures containing PETN. The underestimate in these two cases might result from interaction of the detonation products of PETN with those of lower oxygen components.

The same single HE data were used to obtain D_C values. These in turn were used in Urizar's approximation for D_i. It gave very good results at $\rho_0 = 1.6$ g/cm^3; very poor ones at $\rho_0 = 1.0$ g/cm^3.

Kamlet's approximation for D_i from the H_2O - CO_2 arbitrary decomposition produced values for the mixtures in good agreement with experiment at $\rho_0 = 1.6$ g/cm^3; fair agreement at $\rho_0 = 1.0$ g/cm^3. However, the same procedure resulted in over three percent difference at $\rho_0 = 1.6$ g/cm^3 for two single explosives and in large differences (up to 10%) for four single explosives at $\rho_0 = 1.0$ g/cm^3. The largest differences were for three high oxygen content HE: BTNEU, PETN, and TNETB.

The best overall method for predicting D of mixtures, satisfactory except for high porosity PETN mixtures, is the additivity method of Eq. 17. Its failure in this case is attributed to reaction between the detonation products of PETN and those of oxygen deficient components.

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